REPORT DOCUMENTATION PAGE

Form Approved OMB No 0704-0188

1. AGENCY USE ONLY *(Leave blank)*

2. REPORT DATE 3/13/97

3. REPORT TYPE AND DATES COVERED Final Technical Report 4/1/96 - 9/30/96

4. TITLE AND SUBTITLE Analysis, Design, and Computation of Active Materials

5. FUNDING NUMBERS AF/F49620-96-1-0057

6. AUTHOR(S)

Richard James
Mitchell Luskin

AFOSR-TR-97

0319

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)

University of Minnesota
Grants and Contracts
Office of Research and Technology Transfer Administration
Suite 201
1100 Washington Avenue South
Minneapolis, MN 55415-1226

9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)

AFOSR/NM
Building 410
Bolling AFB, DC 20332-6448

10. SPONSORING/MONITORING AGENCY REPORT NUMBER

11. SUPPLEMENTARY NOTES

12a. DISTRIBUTION/AVAILABILITY STATEMENT

DISTRIBUTION UNLIMITED

12b. DISTRIBUTION CODE

13. ABSTRACT *(Maximum 200 words)*

The research reported here concerns the mathematical modeling and numerical simulation of the behavior of active materials, especially shape memory and magnetostrictive materials. New theories for thin films of active material were derived using change-of-scale calculations. These were used as the basis of several new design concepts for microactuators. Work continued on the modeling of a new class of active materials, magneto-memory materials, whose existence was predicted under previous AFOSR support. Guided by a new theory of magnetostriction, a search has led to the first of these materials during the past year. This material currently exhibits the largest magnetostrictive effect known.

New numerical methods were developed and analyzed for the computation of materials with microstructure. These methods were used to compute the complex microstructure that is observed when a laminate of two phases meets a homogeneous phase.

14. SUBJECT TERMS active materials, shape memory, magnetostrictive, numerical methods

15. NUMBER OF PAGES 5

16. PRICE CODE

17. SECURITY CLASSIFICATION OF REPORT	18. SECURITY CLASSIFICATION OF THIS PAGE	19. SECURITY CLASSIFICATION OF ABSTRACT	20. LIMITATION OF ABSTRACT
UNCLASSIFIED	UNCLASSIFIED	UNCLASSIFIED	UNLIMITED

FINAL TECHNICAL REPORT

AFOSR 49620-96-1-0057
Analysis, Design, and Computation of Active Materials
April 1, 1996 - September 30, 1996

Mitchell Luskin and Richard James
University of Minnesota
March 12, 1997

1 Research Accomplished

James began work on the behavior of thin films of active materials. Using recently developed methods for change-of-scale, he considered the problem of deriving the asymptotically limiting theory for a film of thickness h in the limit as $h \to 0$. These calculations were carried out for general micromagnetics by James and Gioia [6] and for the Ball-James theory of martensite by Bhattacharya and James [2]. The limiting theories give a lot of insight into the energetic role of thinness. They also provide a basis for fast computations on the behavior of active thin films being developed by Luskin and his graduate students.

One of the unexpected results from [2] is that there exist energy minimizing deformations in properly oriented thin films with exact austenite/martensite interfaces, unlike in bulk where austenite/martesite interfaces are always finely twinned (This result also follows from bulk Ball-James theory). These interfaces can be used as a basis of various designs of "tents" and "tunnels" on a thin film which look promising as a basis of large work-output microactuator designs. The theory also says that the current approach which relies on bending (for example, the use of cantilevers) will have significantly less work output. To put these ideas into practice, it will be necessary to make epitaxial thin films of, say, shape-memory or magnetostrictive materials. The authors have persuaded several experimental groups to begin this research (Palmstrøm at Minnesota, Schryvers at RUCA in Belgium), and the work of Palmstrøm along these lines looks promising: the first single crystal thin films of shape memory materials are emerging from this work.

James continued work on magneto-memory materials. These materials, which combine ferromagnetism and shape memory, have been predicted by theory (AFOSR reports, 1992), and the search for these materials has been guided at every stage by modern mathematical theory of transforming materials. During the past year, James and Wuttig have demonstrated field induced strains of 0.5% of certain FePd alloys; these strains are 4-5 times larger than the best giant magnetostrictive materials, so the current materials exhibit the largest known magnetostrictive effect [9]. The design of magneto-mechanical experiments to test these materials was based on a new constrained theory of magnetoelasticity (DeSimone and James).

Luskin gave the first analysis of the approximation of martensitic microstructure for a physically realistic, multi-dimensional crystalline energy [16]. He developed this analysis for the orthorhombic to monoclinic (double well) transformation [16] and then extended the analysis with his graduate student and post-doc, Bo Li, to the cubic to tetragonal (triple well) transformation [12, 14]. They applied the approximation theory developed in his analysis of microstructure to obtain error estimates for the numerical approximation of microstructure by the finite element method. This analysis has given a theoretical basis for the computational program and has made possible the development of more effective and reliable algorithms.

These algorithms have been used by Li and Luskin in computations for mathematical models of material microstructure to explain laboratory results of C. Chu and R. James for microstructured crystals [11, 13]. Their numerical results exhibit the complex microstructure that is observed when a laminate of two phases meets a homogeneous phase. The insights from these computations are very important to the ongoing development of a mathematical theory for martensitic crystals, as well as to the many emerging technologies based on the "shape-memory" property.

Computational experience by Luskin and his collaborators have shown that nonconforming finite element methods (which use deformations that are not required to be globally continuous) can be effective for the computation of crystal microstructure. The rigorous analysis of these elements can be very challenging even for linearly elastic materials. Li and Luskin were able to give a rigorous analysis of the convergence of microstructure for a class of nonconforming finite element methods which validates this method and provides insight that can be used to improve this method [15].

2 Personnel Supported

This grant funded the post-doctoral research of G. Gioia who did research on thin films of magnetostrictive materials and derived the limiting theory for a thin micromagnetic film [6]. Bo Li completed his thesis on the development and analysis of numerical methods for microstructure in active materials and on the complex microstructure that is observed when a laminate of two phases meets a homogeneous phase [11] with the support of this grant, and he continued his research on this project as a post-doctoral researcher with the support of this grant. His publications resulting from work supported by this grant are described above [12, 13, 14, 15]. This grant also partially supported the research of another post-doc, Petr Klouček, on computations of the martensitic transformation [5].

This grant supported the graduate student research of Q. Guo on a new family of composites of shape-memory material. More junior graduate students supported by this grant to work on computational methods for active thin films were Pavel Belik, Tim Brule, and Julia Liakhova.

References

[1] R. Abeyaratne, C. Chu, and R. D. James. Kinetics of materials with wiggly energies: theory and application to the evolution of twinning microstructures in a Cu-Al-Ni shape memory alloy. *Phil. Mag. A*, 73:457–497, 1996.

[2] K. Bhattacharya and R. D. James. Theory of martensitic transformations in thin films. manuscript, 1997.

[3] K. Bhattacharya and R. D. James. Theory of shape-memory thin films with applications. In *MRS Proceedings: Advances in Materials for Smart Systems*, to appear, 1997.

[4] K. Bhattacharya, R. D. James, and P. J. Swart. Relaxation in shape-memory alloys. part I: Mechanical model, part II: Thermomechanical model and proposed experiments. *Acta Materialia*, to appear, 1997.

[5] P. Klouček. Toward the computational modeling of nonequilibrium thermodynamics of the martensitic transformations. Technical Report 1418, IMA, 1996.

[6] G. Gioia and R. D. James. Micromagnetics of very thin films. *Proc. R. Soc. Lond. A*, 453:213–223, 1997.

[7] R. D. James. Wiggly energies. In *Proceedings of the ASME Symposium in honor of J. L. Ericksen, Baltimore, Maryland*, 1996.

[8] R. D. James and H. Tsai. A theory of friction that accounts for the asperities. manuscript, 1997.

[9] R. D. James and Manfred Wuttig. Magnetostriction of martensite. Submitted to Phil. Mag. A, 1997.

[10] Li Jian and R. D. James. Prediction of microstructure in monoclinic $LaNbO_4$ by energy minimization. *Acta Materialia*, to appear, 1997.

[11] Bo Li. *Analysis and computation of martensitic microstructure*. PhD thesis, University of Minnesota, 1996.

[12] Bo Li and Mitchell Luskin. Approximation of a laminate with varying volume fractions. Technical Report 1471, IMA, 1997.

[13] Bo Li and Mitchell Luskin. Numerical simulation of needle-like microstructure in martensitic crystals. manuscript, 1997.

[14] Bo Li and Mitchell Luskin. Finite element analysis of microstructure for the cubic to tetragonal transformation. *SIAM J. Numer. Anal.*, to appear, 1997.

[15] Bo Li and Mitchell Luskin. Nonconforming finite element approximation of crystalline microstructure. *Math. Comp.*, to appear, 1998.

[16] Mitchell Luskin. Approximation of a laminated microstructure for a rotationally invariant, double well energy density. *Numer. Math.*, 75:205–221, 1997.

[17] Mitchell Luskin. Numerical analysis of a microstructure for a rotationally invariant, double well energy. *Zeitschrift für Angewandt Mathematik und Mechanik*, to appear, 1997.